

Dibromomethane
74-95-3 | DTXSID4021557

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 96.7 °C

Global applicability domain: Inside

Local applicability domain index: 6.28e-01

Confidence level: 7.77e-01

Nearest Neighbors from the Training Set

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Dibromomethane

Measured: 97.0

Predicted: 96.7

Image not found

Chloriodomethane

Measured: 109

Predicted: 100

Image not found

Ethane, iodo-

Measured: 72.5

Predicted: 79.1

Image not found

Bromodichloromethane

Measured: 90.0

Predicted: 95.1

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Ethylidene bromide

Measured: 108

Predicted: 109